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Evaluation of the Real-Time Air-Quality Model Using the RAPS (Regional Air Pollution Study) Data Base. Volume 1. Overview

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Menlo Park, CA

Prepared for

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Evaluation of the Real-Time Air-Quality Model Using the RAPS Data Base

Volume 1. Overview

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Volume 1. Overview

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ABSTRACT

The theory and programming of statistical tests for evaluating the Real-Time Air-Quality Model (RAM) using the Regional Air Pollution Study (RAPS) data base are fully documented in four report volumes. Moreover, the tests are generally applicable to other model evaluation problems. Volume 1 presents an overview of the tests, displays, software and application of the resulting statistical package. This report was submitted in fulfillment of Contract No. 68-02-2770 by SRI International under the sponsorship of the U.S. Environmental Protection Agency. This report covers a period from 1 October 1977 to 1 April 1979, and work was completed as of 1 April 1979.

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SECTION 1

INTRODUCTION

BACKGROUND

Until recently, the ability to provide objective evaluations of air quality models has suffered for two reasons. In the first place, adequate test data bases have been scarce, and secondly, the selected statistical procedures have often been inadequate. The first problem has been alleviated somewhat through the acquisition of the extensive Regional Air Pollution Study (RAPS) data base. The primary objective of the RAPS was to provide a data base useful in evaluating, upgrading, and developing air quality models.

With the availability of the comprehensive RAPS data base in mind, EPA retained SRI International to develop a statistical package that would overcome the limitations of currently used statistical procedures. While EPA sought a generally applicable statistical package, they recognized the need to test the package, and for this purpose chose the Real-Time Air-Quality Model (RAM)[1*] along with the RAPS data base.

RAM

The RAM was developed by EPA several years ago as a tool for calculating SO_2 surface concentrations of 1-hour and 24-hour averaging times. These can be used to form estimates of SO_2 concentrations for 3-hour, monthly, seasonal, and annual averaging times. This Gaussian-plume multiple-source (point and area) model requires hourly input data for emissions and meteorological parameters from a single site. Hence, the model output consists of an SO_2 concentration prediction for each hour.

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*References are listed at the end of this report.

RAPS Data Base

The RAPS was conducted in St. Louis because that geographic area already had a fairly good historic air quality data base and was one of the least complicated urban areas to model. (St. Louis has fairly level terrain and is free of pollutant intrusion from other large urban areas.) The heart of the RAPS is the 25-station air-monitoring network that collects data on the criteria pollutants (including SO_2) and meteorological parameters (wind, ambient temperature, dew point temperature, and temperature gradient). In addition, numerous special measurements were made at the monitoring sites, other surface locations, and aloft. Hence, the data base is rich not only in the SO_2 measurements needed to evaluate model performance, but also in the emission and meteorological measurements needed to understand the limitations of the RAM input parameters.

OBJECTIVES

The overall objective of this research is the implementation of a computer-based statistical package useful in both evaluating model performance and gaining insight into the causes of poor performance. Specific goals of the delivered statistical package (software and reports) include the following:

- Figures of merit (or scores) that describe the absolute accuracy, temporal distribution, and some spatial features of the compared parameters (observed versus predicted concentrations).
- Techniques that enable one to relate such figures of merit to the model input parameters.
- Auxiliary displays that allow one to visualize the significance of the figures of merit.
- Software compatible to the EPA Univac 1110 and readily applicable to the evaluation of the RAM using the RAPS data base.
- Complete documentation that allows one to adapt the package to any air quality model evaluation problem, with a special emphasis on the RAM evaluation.

Because the complete RAPS data base was not ready for use in time, the actual application of the developed package to the RAM evaluation was not the immediate goal of this research. A special test data base

described later was used to check the software package. However, application to the RAM evaluation is the immediate goal of follow-through research.

SECTION 2

OVERVIEW

GENERAL APPROACH

The main project work elements are identified in the flow chart of Figure 1. Basically, the general approach was formulated in the proposal but was modified slightly because essential parts of the RAPS data base were not immediately available. The RAPS air-quality data were still undergoing quality assurance checks, and the emissions data base was not ready for input to the RAM. Consequently, it was necessary to select a different test data base.

The test data base was acquired in a recent SRI tracer study.[2] This data base is summarized in Appendix A. While it would have been more efficient to work with a segment of the RAPS data base, the test data base offered the following advantages:

- It had previously been analyzed, so some of the results from our newly programmed techniques could be corroborated.
- A limited but well-defined set of meteorological model input parameters is part of the data base, so model performance could be evaluated as a function of these parameters.

Concurrent with the selection of the test data base, many statistical techniques were considered for inclusion in a recommended statistical evaluation package. Essentially, all recommended tests and auxiliary displays were implemented in six distinct computer programs which were tested and documented.

As shown in Figure 1, a second phase consists of adaptation of the statistical package to the RAM evaluation problem, using the RAPS data base.

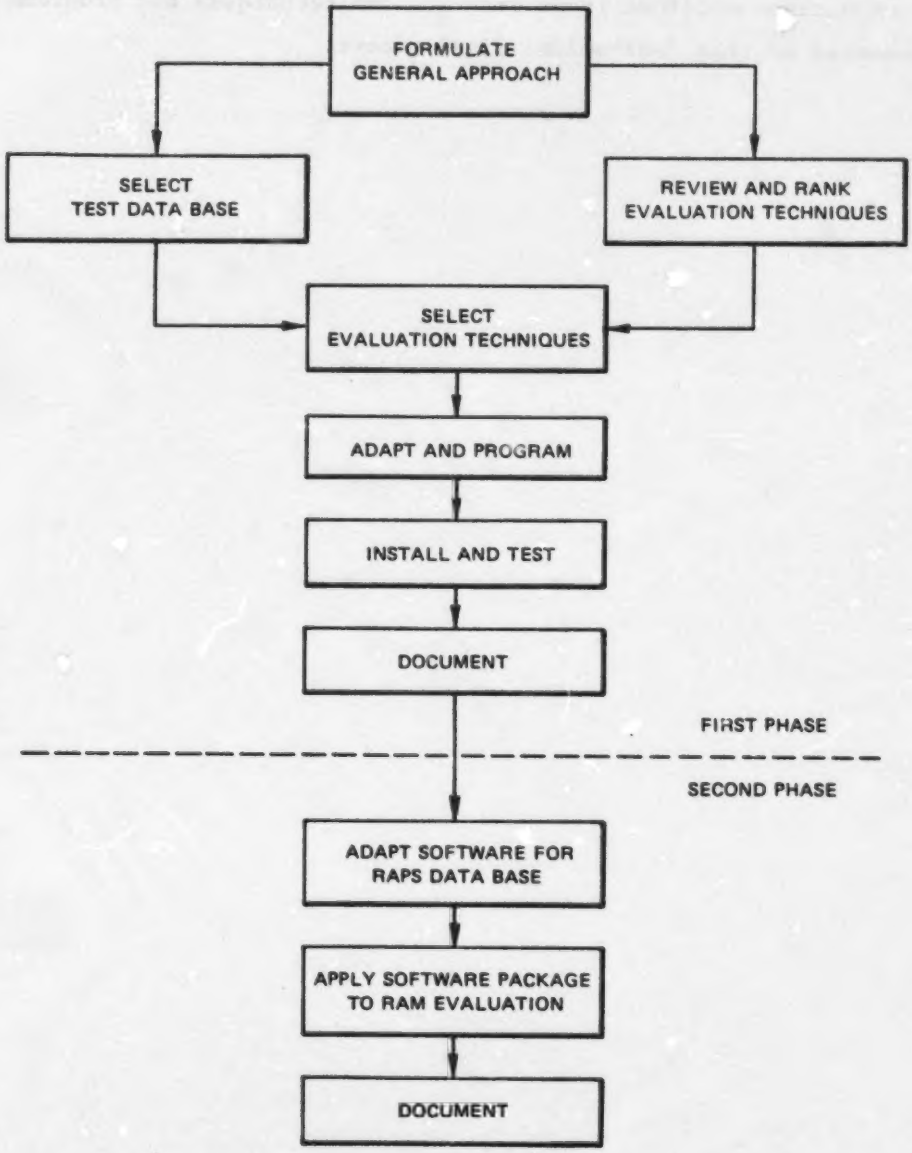

Figure 1. Project flow chart.

ACCOMPLISHMENTS

Six statistical programs were developed, installed on the EPA Univac 1110, and successfully tested. In general, the combined programs meet the the objectives outlined in Section 1. The techniques and programs are documented in this four-volume final report.

SECTION 3

TECHNICAL SUMMARY

PREVIEW

Six statistical programs have been developed for the purposes of model evaluation. A distinction is made between a "final-evaluation" statistic and an "intermediate-evaluation" statistic. The first program--accuracy score--evaluates the performance of the model, and as a final evaluation statistic is considered the bottom-line computation. The remaining five tests are intermediate-evaluation statistics that are meant to assist one in the diagnosis of the causes of poor model performance.

Most of the programs contain auxiliary display software that allows the user to visualize the results as an aid to determining the meaning of the numerical output. Each program was installed and tested on the EPA Univac 1110 computer system in Research Triangle Park, North Carolina. A Tektronix 4014 terminal was used for graphic outputs.

The following subsections summarize the statistical tests, the rationale behind their selection, the auxiliary displays. the software, and evaluation procedures, which are described more comprehensively in Volumes 2 and 4 of this report.

SELECTION OF STATISTICAL TESTS

In Volume 2 we consider a number of statistical tests for the purposes of final evaluation and intermediate evaluation. (It is noted that there is often some interchangeability between tests used for both purposes.)

Final Evaluation

Various loss functions were implemented as a final-evaluation statistic. These were termed Accuracy Scores. The Accuracy Score program is applied to a data base of observed and predicted concentrations. As

the difference between observation and prediction decreases, so does the Accuracy Score. Hence, Accuracy Score is like a golf score--the lower, the better.

The following eight Accuracy Score tests are recommended:

- Average absolute error
- Average squared error
- Percent incorrect predictions above an absolute error threshold
- Percent incorrect prediction above a constant percentage error threshold
- Symmetric high-low loss function
- Asymmetric high-low loss function
- User-supplied loss matrix
- Location of maximum concentration.

The first seven accuracy scores are concerned with errors in prediction both for a given location and for the composite at all locations. The eighth accuracy score is concerned with losses due to an error in predicting the location of the maximum observed concentration.

For the first two loss functions, calculation of the accuracy score is straightforward from the objective comparison of observed and predicted concentrations. The third through fifth tests require entry of a user-supplied threshold value. For cases when agreement between observation and prediction is within the threshold value, a loss of zero is assigned; otherwise, the loss is 1. The sixth and seventh tests again use the threshold concept, but assign subjectively derived loss values supplied by the user. (Hence, in these cases, the user can determine the types of disagreement that are most important and weight them accordingly.) The eighth test also uses user-supplied loss values that typically are proportional to the distance between the location of the observed maximum and the location of the predicted maximum.

The output of each test is a score that is the summation of scores of each individual comparison. In addition, confidence limits for the accuracy score are computed. As a software option, the user can display the accuracy scores on a geographical map. Then the spatial trends in prediction accuracy can be assessed.

Intermediate Evaluation

A number of statistical tests were considered for the purpose of intermediate evaluation. (As noted in Volume 2, there are special cases where these tests can also be used as a final evaluation tool.) The following tests and displays are recommended and included as part of the software package:

- Scatter plot
- Linear regression with confidence and prediction bands
- Pearson's correlation coefficient
- Chi-square test and frequency distribution displays
- Interstation error correlation
- Multiple regression of error residuals
- Analysis of residual time series.

In the software package, as discussed later, some of the above tests were combined to make computer execution more efficient. In the following paragraphs, the tests are considered separately.

A simple scatterplot, also known as a scattergram, is one of the most useful evaluation tools because it displays a case-by-case comparison of all data (i.e., observed versus predicted concentrations). A regression analysis can be added to compute and display (on the scatterplot) a least-squares fit of the data. Confidence and probability bands can be calculated and added to the display to demonstrate the statistical significance of the regression (least squares) line and the probability of a new test point falling outside the bands, respectively. The Pearson's correlation coefficient is calculated as a measure of how linear the comparison is.

The chi square test and accompanying frequency distribution display are a measure of how well the predicted frequency distribution agrees with the observed frequency distribution. This test is also a useful final evaluation statistic when the distribution itself is important and not the point-by-point comparison.

The interstation error correlation tests examines the correlation between station errors. (Error is the difference between observed and predicted concentrations.) This test is useful for identifying geographical (or spatial) bias in the model comparison process. Correlation of the error (residuals) with the model input parameters is computed by the multiple regression of error residuals test. The primary purpose of this test is to diagnose which of the input parameters most influence the model's poor performance. The analysis of residual time series test examines the errors for any cyclical behavior. It determines whether errors occur on a periodic basis and what the time period is.

STATISTICAL AND DISPLAY SOFTWARE

The statistical tests and associated displays mentioned in this section were programmed, debugged, and tested. The Pearson's correlation coefficient and linear regression tests (with scatterplot showing confidance and prediction bands) were combined into one test named "bivariate regression and correlation". Thus, the six individual programs have test names as follows:

- Accuracy Score
- Residual Time Series
- Chi-square Goodness of Fit
- Bivariate Regression and Correlation
- Interstation Error Correlation
- Multiple Regression of Error Residuals.

The first five programs were written in the FORTRAN V programming language. The last test was written in the specialized SPSS language.[3]

Auxiliary programs were written or converted to complement the statistical tests. Several SPSS procedures were written to sort, retrieve, and display selected portions of the data base. Also, to assist the evaluator in visualizing differences between the observed and predicted concentrations, programs to display the frequency distributions on a logarithm-probability axis are included in the package.

The software has some special features unique to the EPA Univac 1110 computer system and EPA-supported software for the Tektronix 4014 graphics terminal. However, the programs are generally compatible with software supported on most major computers and are therefore easily convertible. The software is fully documented in Volume 3 of this final report.

EVALUATION OF THE RAM

The general method of applying the statistical and display programs remains essentially the same regardless of the specific air-quality model being tested. To adapt the programs to the RAM evaluation, only minor software changes must be made.

Evaluation of a model requires the following steps:

- Preparation and analysis of the data base
- Selection of the specific data set of interest
- Selection and application of the statistical test
- Interpretation of the test results.

These steps are repeated in an iterative fashion. As test results are analyzed, the evaluator tries another test and so forth until full value has been garnered from the statistical tests.

As noted in Volume 4 of this report, when evaluating the RAM, one or more specific indicators of poor performance are looked for. These include:

- General bias occurs when the differences in observed and predicted concentrations are mostly of the same magnitude and sign. Several of the tests will detect this condition.
- Spatial bias is similar to general bias, differing in that the patterns are examined for individual monitoring stations. The

same tests for general bias are applicable here, but they are applied to each site. In addition, the interstation error correlation test is useful in addressing error residuals and then spatial pattern.

- Temporal (cyclic) bias is detectable by the residual time series test. Temporal bias is indicated when the errors in misprediction are periodic.
- Randomness is indicated when poor agreement exists (between observed and predicted concentrations) and there is no apparent trend. This is best displayed in the bivariate regression and correlation program--visually with the scatterplot and numerically with a low Pearson's correlation coefficient.
- Input-parameter dependence exists when poor performance can be traced to one or more of the input parameters. The multiple regressions of error residuals test is useful for this purpose. Other tests, applied to subsets of the data base, can also be effective in detecting input parameter dependence.

The tests are able to detect all of the above indicators of poor model performance. Guidelines in their applications are presented in Volume 4.

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3. N. H. Nie, C. H. Hull, J. G. Jenkins, K. Steinbrenner, D. H. Bent, Statistical Package for the Social Sciences (McGraw-Hill Book Co., New York, New York, 1975).

APPENDIX A

DESCRIPTION OF THE TEST DATA BASE

OVERVIEW

During the fall, 1974, a series of diffusion tests was conducted by SRI International (then Stanford Research Institute) at Millstone Nuclear Power Station in southeastern Connecticut under sponsorship of the Atomic Industrial Forum (AIF) and the Northeast Utilities Service Company (NUSCO). This field study was planned by the AIF as part of its program for evaluating roof-vent effluent diffusion from reactor and turbine buildings.

The goal of the overall program was to develop and validate a more realistic general model than was currently available for calculating annual-average concentrations resulting from effluent diffusion from roof vents. The limited objectives of the Millstone field study were to:

- Collect data sufficient to describe the diffusion of effluents from the Millstone reactor and turbine building roof vents, especially under conditions of low wind speed.
- Use these data to develop and validate a site-specific diffusion model for calculating annual-average concentrations.
- Evaluate the suitability of the planned experimental design for an overall test program.

To collect the necessary data, diffusion tests were conducted, during which sulfur hexafluoride (SF_6) tracer gas was released from the reactor building main vent and dibromodifluoromethane (Freon-12B2) from three of the ten turbine building vents. Air samples were collected by sequential multiple-bag samplers at 44 locations on three concentric 88-deg arcs at distances of 350, 800, and 1500 m from the SF_6 release point. The air samples were analyzed by gas chromatography to obtain downwind concentrations of the tracer gases.

A visible oil-fog tracer was also injected into the reactor building vent, and the resulting plume was photographed by two orthogonally positioned time-lapse cameras.

Supplementary special observations included three-component wind measurements at three locations above the reactor and turbine building roofs, and vent efflux speed and temperature excess on both buildings. A complete set of meteorological measurements at heights up to 137 m above the ground was also available at the site from the existing NUSCO instrumented tower.

Data from a total of 36 hour-average runs were available. These data were compared with the predictions of current models endorsed by the U.S. Nuclear Regulatory Commission (NRC).* In addition, the data were used to develop and validate a realistic annual-average model, the "Split-H" model.

The "Split-H" model takes account of the observed relationship between the degree of plume entrainment and the velocity ratio (U_e/U), where U_e is the vent efflux velocity and U is the wind velocity. The name "Split-H" was given because the model divides concentrations at a receptor into both a wake entrainment component coming from ground level ($H = 0$), and a liftoff component coming from the effective vent height ($H = H_e$). The respective weighting of these components is taken to be a function of U_e/U.

MILLSTONE SITE CHARACTERISTICS PLANT CONFIGURATION AND INSTRUMENT LAYOUT

The Millstone Nuclear Power Station is located in Waterford, Connecticut, on the tip of a small peninsula that extends southward into Long Island Sound. The land rises gradually from the shore to reach a maximum elevation of 100 ft (30 m) above mean sea level along the northern edge of the test area. Approximately 30 percent of the test area is

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*Formerly the U.S. Atomic Energy Commission (AEC).

wooded, composed mostly of deciduous trees. The remaining area has been cleared and consists of brush and pasture land.

Millstone Station is currently composed of two electric generating units, Units 1 and 2. At the time of the field study, Unit 2 was still under construction, but all the external structures had been completed. In addition, excavations had begun for a third unit. Testing was confined to the reactor and turbine building roof vents of Unit 2. Meteorological measurements at five different levels were available from the 137-m NUSCO tower located 500 m SSE of the Unit 2 reactor building vent (see Figure A-1).

The original experimental design contained in the General Test Plan called for a 180-deg array of bag samplers on at least two arcs. This layout had to be modified for the Millstone study because of the constraints imposed by the surrounding waters of Long Island Sound. The instrumentation layout that was adopted during the field tests consisted of 45 samplers located at 40 stations arranged on three arcs extending out to 1500 m, plus an upwind background station, as depicted in Figure A-2. Five samplers were elevated at a height of 25 m by means of towers uniformly spaced along the outer arc.

TEST RESULTS

Table A-1 presents the relevant data from each of the 36 analyzed SF_6 runs. As indicated, the Pasquill stability classes (A through G) were derived by using temperature differences (ΔT) between two sets of heights. The scheme, called S_1, uses the observed ΔT between the 137-m and 10-m levels, while the S_2 scheme uses the ΔT between 43 m and 10 m. The concentrations (χ) were normalized with respect to wind speed (U) and source strength (Q). Other variables in the table are wind direction (θ) and efflux velocity (U_e).

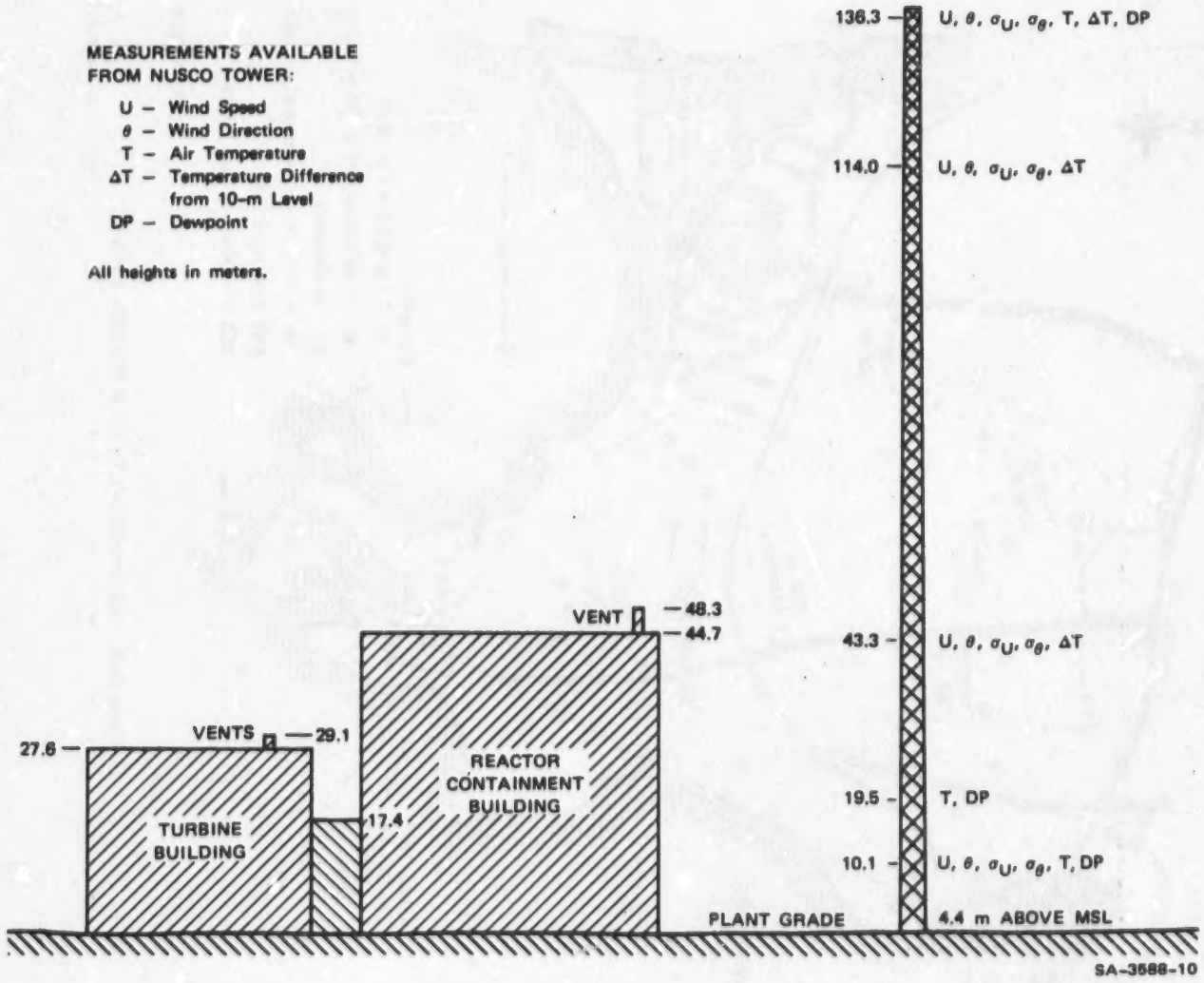


Figure A-1. Vertical profile of Millstone Unit 2 and NUSCO meteorological tower, looking 344°.

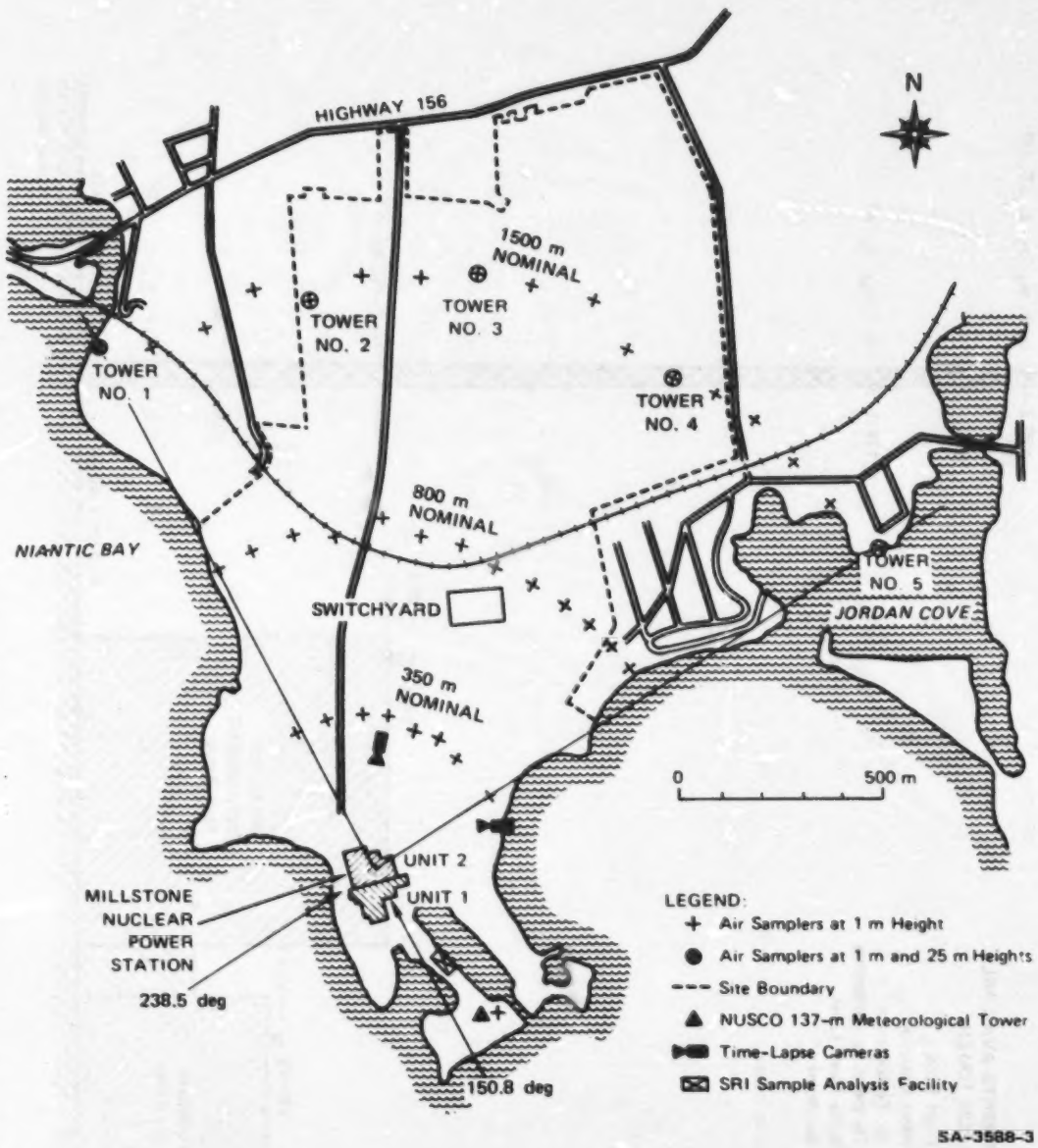


Figure A-2. Instrumentation layout at Millstone station.

TABLE A-1. SUMMARY OF MILLSTONE SF_6 TRACER DATA

Run Number	Date (1974)	Start Time*	θ (deg)	U (m/s)	U_e (m/s)	U_e/U	Stability Data† (deg C/100 m) ΔT_1	ΔT_2	S_1	S_2	Normalized Centerline Concentration‡ $\chi U/Q$ (10^{-6} m^{-2}) X = 350 m Obs.	Calc. (S_1)	Calc. (S_2)	X = 800 m Obs.	Calc. (S_1)	Calc. (S_2)	X = 1500 m Obs.	Calc. (S_1)	Calc. (S_2)
1	12 Oct	0900	206	7.8	8.7	1.11	-1.2	-2.0	D	D	310	464	464	130	174	174	41	70	70
2	↓	1000	210	7.2	↓	1.21	-1.3	-1.8	↓	D	230	↓	464	108	↓	174	67	↓	70
3		1100	209	7.1		1.22	-1.3	-2.5		A	216		60	70		6	25		1
4		1200	215	7.8		1.12	-1.2	-2.1		C	221		253	97		70	44		24
5	14 Oct	1000	148	6.4	8.3	1.30	-1.4	-2.6		A	107		60	40		6	11		1
6	↓	1100	150	5.9	↓	1.41	-1.4	-2.6	↓	A	129	↓	60	39	↓	6	8	↓	1
8	15 Oct	0900	212	9.2	8.1	0.88	-0.3	-0.5	E	E	230	625	625	40	287	287	52	134	134
9	↓	1000	230	7.5	↓	1.08	-0.2	-0.1	↓	↓	262	↓	↓	256	↓	↓	30	↓	↓
10		1100	233	8.6		0.94	0.0	-0.1			269			856			62		
11	25 Oct	0800	197	8.5	8.7	1.02	-1.2	-1.8	D	D	477	464	464	169	174	174	69	70	70
12	↓	0900	192	9.1	↓	0.96	-1.2	-2.1	↓	C	465	↓	253	141	↓	70	36	↓	24
13		1000	198	9.1		0.96	-1.2	-2.0		D	411		464	164		174	32		70
14		1100	203	10.8		0.81	-1.2	-1.8		↓	487		↓	147		↓	44		↓
15		1200	204	11.7		0.74	-1.2	-1.8			359			157			73		
16		1300	198	11.4		0.76	-1.1	-1.7			499			186			72		
17		1400	203	11.7		0.74	-1.1	-1.8			442			196			41		
18	↓	1500	208	11.4	↓	0.76	-1.1	-1.6	↓	↓	313	↓	↓	141	↓	↓	49**	↓	↓
28	31 Oct	1700	203	3.7	4.8	1.30	0.4	1.2	E	E	195	625	625	40	287	287	24**	134	134
29	↓	1800	215	4.5	4.6	1.02	-0.1	-0.8	E	E	207	625	625	18	287	287	26	134	134
30		1900	217	3.3		1.39	-0.7	-1.2	D	D	119	464	464	73	174	174	23	70	70
31		2000	224	3.4		1.35	-0.4	-1.2	E		201	625	↓	77	287	↓	39	134	↓
32	↓	2100	228	3.6	↓	1.28	-0.2	-1.2	E	↓	138	625		137§	287		34	134	
36	4 Nov	0700	229	5.1	5.8	1.14	-0.7	-1.5	D		86§	464	↓	48§	174	↓	17	70	↓
45	14 Nov	0300	199	7.6	8.6	1.13	-1.1	-1.8	↓	↓	331	↓		153	↓		59	↓	
46	↓	0400	189	8.6	↓	1.00	-1.2	-2.1		C	569	↓	253	140	↓	70	61	↓	24
47		0500	197	10.3		0.83	-1.2	-2.3		B	598		121	170		28	52		8
48		0600	197	10.1		0.85	-1.2	-1.8		D	434		464	157		174	55		70
49		0700	192	10.3		0.83	-1.2	-2.0		↓	467		↓	146		↓	53		↓
50		0800	193	10.7		0.80	-1.2	-1.8			470			164			41		
51		0900	190	11.3		0.76	-1.2	-1.8			520			134			56		
52		1000	187	12.5		0.69	-1.1	-1.8			463			170			55		
53		1100	185	12.4		0.69	-1.1	-1.7			454			162			58		
54	↓	1200	184	12.4	↓	0.69	-1.1	-1.7	↓	↓	539	↓	↓	161	↓	↓	54	↓	↓
57	20 Nov	0200	176	4.3	8.6	2.00	-1.1	-1.8			73			75			29		
58	↓	0300	153	4.0	↓	2.15	-1.0	-1.8			65			50			12**		
59		0400	151	4.0		2.15	-1.1	-1.8	↓	↓	37	↓	↓	23	↓	↓	8**	↓	↓

*EDT, becoming EST on 27 October.

†$\Delta T_1 = (T_{137\ m} - T_{10\ m})/1.27$; $\Delta T_2 = (T_{43\ m} - T_{10\ m})/0.33$; S_1 and S_2 are NRC stability classes corresponding to ΔT_1 and ΔT_2.

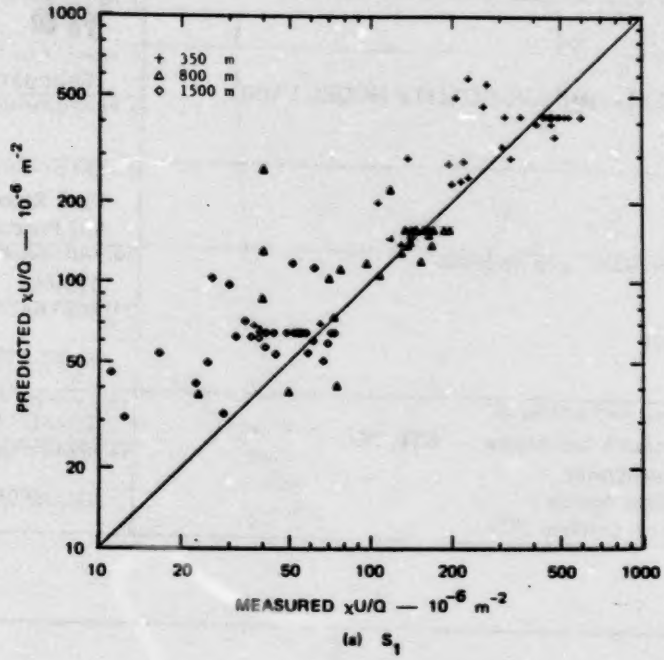
‡Calculated concentration values are based upon the NRC accident model.

§Value not included in analysis because plume centerline may be off sampling grid.

**Value not included in analysis because sampler location where maximum was observed is judged to be off-centerline to a significant degree.

VALIDATION OF THE "SPLIT-H" MODEL

Figure A-3 compares the measured normalized-centerline tracer concentrations with those predicted by the "Split-H" model for the two different stability classification schemes, S_1 and S_2. (The test data base for the RAM evaluation uses only the S_1 version. The distinction among the radial distances--350 m, 800 m, and 1500 m--serves as an analog to a distinction among monitoring sites--labeled 1, 2, and 3 in the test data base.)



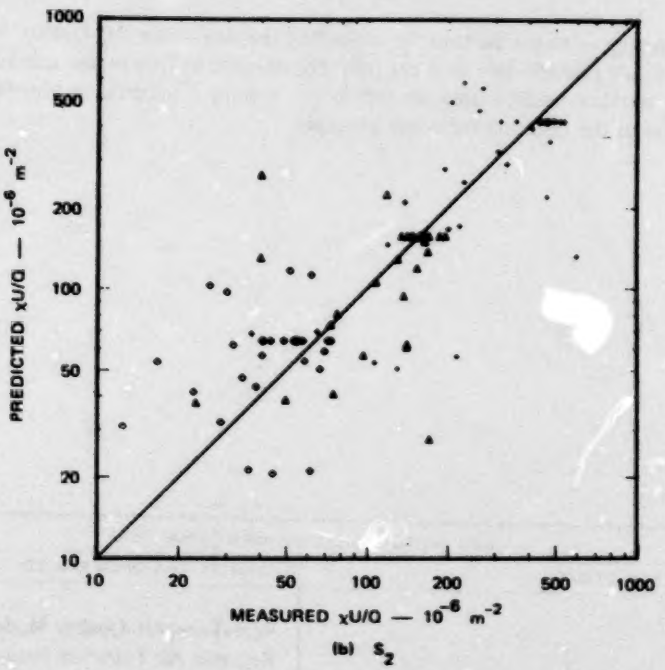


Figure A-3. Comparison between observed normalized centerline concentrations and those predicted by the split-H model for S_1 and S_2 stability classification criteria.